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Multivariate Calibration: A Generalization of the Classical Estimator

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In univariate calibration problems two different estimators are commonly in use. They are referred to as the classical estimator and the inverse estimator. Krutchkoff (1967, *Technometrics* **9**, No. 3 425–439) compared these two methods of calibration by means of an extensive Monte Carlo study. Without mathematical proof he concluded that the classical estimator has a uniformly greater mean squared error than the inverse estimator. Krutchkoff's paper resulted in an immediate controversy on the subject of his criterion, for the classical estimator has an infinite mean and mean squared error. In this paper we consider a generalization of the classical estimator for multivariate regression problems. We show that this estimator has a finite mean if the dimension, say p, of the response variable is greater than 2, and we show that the mean squared error is finite if p is greater than 4. We also give exact expressions for the mean and the mean squared error in terms of expectations of Poisson variables, which can be easily approximated.

1. Introduction and Examples

In a multivariate calibration problem we consider an initial sample $(\mathbf{Y}_i, x_i)$; $i = 1, 2, ..., n$ $(n \geqslant 2)$, where $\mathbf{Y}_i$ is a p-dimensional vector of observations. The $\mathbf{Y}_i$ are assumed to be independently normally distributed random vectors with common covariance matrix $\boldsymbol{\Sigma}$. The x_i are known constants (chosen), values of a controlled variable x, at least two of which are distinct.

We assume that it has already been determined that the elements of the response vector $\mathbf{Y}$ are linearly related to x. Thus we have a multivariate linear regression model involving a single nonrandom predictor variable x. P. J. Brown [4] examined more general multivariate calibration problems

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with multiple linear regression models and random x, but in this paper the model is the simplest linear regression model, denoted by

$$\mathbf{Y}_i \sim N_p(\boldsymbol{\alpha} + \boldsymbol{\beta} x_i, \boldsymbol{\Sigma}); \qquad i = 1, 2, ..., n, \tag{1.1}$$

where

$$\mathbf{Y}_i = (Y_{i1} Y_{i2} \cdots Y_{ip})',$$
$$\boldsymbol{\alpha} = (\alpha_1 \alpha_2 \cdots \alpha_p)',$$
$$\boldsymbol{\beta} = (\beta_1 \beta_2 \cdots \beta_p)'.$$

We shall refer to the initial sample as the calibration experiment. Suppose a new measurement $\mathbf{Y}_0 = (Y_{01} Y_{02} \cdots Y_{0p})'$ is obtained at an unknown value x_0 of x. It is assumed that model (1.1) above is also valid for $\mathbf{Y}_0$, and that $\mathbf{Y}_0$ is independent of the observations in the calibration experiment. The main purpose of calibration is to estimate x_0.

We encountered the multivariate calibration problem in a biological study by Broekhuizen and Maaskamp [2] on the age determination of hares. The age of a hare found dead in the open field can be determined from several criteria, for example, body weight, eye lens weight, and length of the hind foot. Observations concerning these criteria suggest linear relationships between the various criteria and age (on a log scale). Thus a multivariate regression model could be assumed, at least within a certain age interval. From a calibration experiment involving a number of hares of known ages the model parameters could be estimated. Subsequently, the unknown age x_0 of a dead hare could be estimated on the basis of the vector of measured criteria $\mathbf{Y}_0$ and the results of the calibration experiment. Similar examples are reported by Oman and Wax [11] and G. H. Brown [3].

The common estimators $\mathbf{a}$ and $\mathbf{b}$ for $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, based on the calibration experiment, are

$$\mathbf{a} = \bar{\mathbf{Y}} - \mathbf{b}\bar{x}, \tag{1.2}$$

$$\mathbf{b} = \sum_i (x_i - \bar{x})(\mathbf{Y}_i - \bar{\mathbf{Y}})/C, \tag{1.3}$$

where

$$\bar{\mathbf{Y}} = \sum_i \mathbf{Y}_i/n,$$

$$\bar{x} = \sum_i x_i/n, \tag{1.4}$$

$$C = \sum (x_i - \bar{x})^2.$$

As regards model (1.1), $\mathbf{a}$ and $\mathbf{b}$ are maximum likelihood estimators. In a practical situation we also need an estimator for $\boldsymbol{\Sigma}$, and an appropriate choice would be the maximum likelihood estimator $\mathbf{S}$ given by

$$\mathbf{S} = \sum_i (\mathbf{Y}_i - \mathbf{a} - \mathbf{b}x_i)(\mathbf{Y}_i - \mathbf{a} - \mathbf{b}x_i)'/n. \tag{1.5}$$

In this paper we assume that the matrix $\boldsymbol{\Sigma}$ is known. This is simply done to reduce the magnitude of the problem, which is in itself already very complex. We also assume that $\boldsymbol{\Sigma}$ is positive definite, hence there exists a symmetric matrix $\boldsymbol{\Sigma}^{1/2}$ such that $\boldsymbol{\Sigma}$ can be written as $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^{1/2}\boldsymbol{\Sigma}^{1/2}$. We confine ourselves to a situation where there is only one new observation $\mathbf{Y}_0$ at the unknown x_0, because we do not include consistency problems in this paper. However, the results are easily adapted for a situation of, say, k observations at x_0.

2. A Generalization of the Classical Estimator

After having estimated $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ by $\mathbf{a}$ and $\mathbf{b}$ we consider the expression

$$\mathbf{Y} = \mathbf{a} + \mathbf{b}x, \tag{2.1}$$

which represents the estimated linear relationships between the p elements of the response vector $\mathbf{Y}$ and the variable x.

Suppose a new measurement $\mathbf{Y}_0$ is available at the unknown value x_0 of x. In the univariate case ($p = 1$) the parameter x_0 can be estimated by solving the equation $Y_0 - a - bx_0 = 0$. This gives the usual classical estimator in calibration problems [5]

$$\hat{x}_0 = \frac{Y_0 - a}{b}. \tag{2.2}$$

In a multivariate calibration problem, however, this approach would lead to a system of p equations of the form

$$Y_{0j} - a_j - b_j x_0 = 0; \qquad j = 1, 2, ..., p, \tag{2.3}$$

and it is unlikely that this system has a solution, due to the random character of the vector $\mathbf{Y}_0$.

A natural way to estimate x_0 is to minimize the quantity

$$(\mathbf{Y}_0 - \mathbf{a} - \mathbf{b}x_0)' \, \boldsymbol{\Sigma}^{-1}(\mathbf{Y}_0 - \mathbf{a} - \mathbf{b}x_0). \tag{2.4}$$

Differentiation to x_0 gives a generalization of the classical estimator, defined by

$$\hat{x}_0 = \frac{(\mathbf{Y}_0 - \mathbf{a})' \boldsymbol{\Sigma}^{-1} \mathbf{b}}{\mathbf{b}' \boldsymbol{\Sigma}^{-1} \mathbf{b}}. \tag{2.5}$$

This is not the only possible generalization, because other convenient matrices might be inserted in (2.4) instead of $\boldsymbol{\Sigma}$. However, the choice of $\boldsymbol{\Sigma}$ is obvious. It is also applied in the concept of "best linear estimation" introduced by Lewis and Odell [10] in 1966. They consider estimation problems for arbitrary dimension q of x_0. When $q \leqslant p$ and $\mathbf{b}$ is known their estimator is the generalization of (2.5) for multidimensional x_0. In the context of calibration G. H. Brown [3] already mentioned formula (2.5) in 1979 in a concise appendix at the end of his paper. P. J. Brown [4] and Fujikoshi and Nishii [6] discuss the construction of confidence intervals for multidimensional x_0.

It is interesting to note that $\hat{x}_0$ is a weighted sum of the solutions of Eq. (2.3), where the jth solution is multiplied by the weight

$$\frac{(0 \cdots 0 b_j 0 \cdots 0) \boldsymbol{\Sigma}^{-1} \mathbf{b}}{\mathbf{b}' \boldsymbol{\Sigma}^{-1} \mathbf{b}}. \tag{2.6}$$

Since a_j and b_j coincide with the univariate estimators for α_j and β_j if we separately consider the jth response in the sample, the estimator (2.5) can be written as a weighted sum of the univariate classical estimators for the distinct responses.

The concept of inverse estimation [8] can also be extended to multivariate observations. Then the following sum of squares is minimized

$$\sum_i (x_i - \gamma - \boldsymbol{\delta}' \mathbf{Y}_i)^2, \tag{2.7}$$

where γ is a scalar and $\boldsymbol{\delta} = (\delta_1\ \delta_2 \cdots \delta_p)'$. The resulting estimators for γ and $\boldsymbol{\delta}$, say g and $\mathbf{d}$, can be used to define the inverse estimator $\tilde{x}_0$ as

$$\tilde{x}_0 = g + \mathbf{d}' \mathbf{Y}_0. \tag{2.8}$$

As this paper is concerned with the classical estimator, the details of the calculation of g and $\mathbf{d}$ are excluded.

In 1967 a long controversy concerning the univariate classical estimator arose, following a Monte Carlo study by Krutchkoff [8], in which he compared the classical estimator and the inverse estimator. For obvious reasons Krutchkoff excluded a small interval around zero for the b values in his computations. Therefore he found finite results for the mean and the mean squared error of the classical estimator adapted in this way, although these characteristics are infinite in expectation for the unadapted estimator. On the other hand, Taylor expansions for the mean and the mean squared error give finite results, as Shukla [13] showed.

In this confusing situation the mean squared error was rejected as a criterion for comparison of the classical and the inverse estimator. Halperin [7] proposed the use of Pitman's closeness, and afterwards Krutchkoff [9] revised his conclusions.

In this paper it is shown that this confusing situation does not occur if the dimension of the observations is greater than 4. Thus in multivariate calibration problems, the mean squared error might be a good criterion for comparison. It would be interesting to compare the exact results given in Section 7 of this paper, which are in terms of Poisson variables, with corresponding exact results for the multivariate inverse estimator. However, at the time of this writing, this question was still under investigation. For the univariate inverse estimator the mean squared error has recently been expressed by Oman [12]. In his formula, Poisson variables also appear.

3. Reparametrization

In order to examine the first and second moment of the generalization of the classical estimator (2.5), we introduce two vectors $\mathbf{T} = (T_1 T_2 \cdots T_p)'$ and $\mathbf{U} = (U_1 U_2 \cdots U_p)'$ defined by

$$\mathbf{T} = \boldsymbol{\Sigma}^{-1/2}\mathbf{b}C^{1/2}, \tag{3.1}$$

$$\mathbf{U} = \boldsymbol{\Sigma}^{-1/2}(\mathbf{Y}_0 - \bar{\mathbf{Y}})\frac{n^{1/2}}{(n+1)^{1/2}}. \tag{3.2}$$

It is well known from regression theory that $\mathbf{T}$ and $\mathbf{U}$ are independent. Furthermore, multiplication by the matrix $\boldsymbol{\Sigma}^{-1/2}$ and the constants, where C is defined in (1.4), and n is the number of observations in the calibration experiment, gives $\mathbf{T}$ and $\mathbf{U}$ spherical normal distributions, i.e., covariance matrix $\mathbf{I}_p$.

The vector of means $\boldsymbol{\tau} = (\tau_1 \tau_2 \cdots \tau_p)'$ corresponding to $\mathbf{T}$ is

$$\boldsymbol{\tau} = \boldsymbol{\Sigma}^{-1/2}\boldsymbol{\beta}C^{1/2}. \tag{3.3}$$

If we finally introduce the parameter X_0 defined by

$$X_0 = \frac{x_0 - \bar{x}}{C^{1/2}}\frac{n^{1/2}}{(n+1)^{1/2}}, \tag{3.4}$$

the distributions of $\mathbf{T}$ and $\mathbf{U}$ are

$$\mathbf{T} \sim N_p(\boldsymbol{\tau}, \mathbf{I}_p), \tag{3.5}$$

$$\mathbf{U} \sim N_p(X_0\, \boldsymbol{\tau}, \mathbf{I}_p). \tag{3.6}$$

After substitution of (1.2), (3.1), and (3.2) in (2.5) we find the estimator $\hat{X}_0$ for X_0

$$\hat{X}_0 = \frac{\mathbf{U}'\mathbf{T}}{\|\mathbf{T}\|^2}, \tag{3.7}$$

where $\|\mathbf{T}\|^2 = \mathbf{T}'\mathbf{T} = \sum_i T_i^2$.

It is clear that estimation of X_0 is equivalent to estimation of x_0, and in the next sections we focus our attention mainly on X_0. We shall return to x_0 in Section 7.

4. Preliminary Results

Since $\mathbf{T}$ and $\mathbf{U}$ are independent, the mean of the estimator $\hat{X}_0$ defined in (3.7) can be shown as a product of means, where the mean of $\mathbf{U}$ is given in (3.6).

$$\begin{aligned} E\{\hat{X}_0\} &= E\{\mathbf{U}\}'\, E\left\{\frac{\mathbf{T}}{\|\mathbf{T}\|^2}\right\} \\ &= X_0\, \boldsymbol{\tau}' E\left\{\frac{\mathbf{T}}{\|\mathbf{T}\|^2}\right\}. \end{aligned} \tag{4.1}$$

Also with $\operatorname{tr}(\cdot)$ being the trace of a matrix, the second moment is as follows

$$\begin{aligned} E\{\hat{X}_0^2\} &= E\left\{\frac{\mathbf{U}'\mathbf{T}}{\|\mathbf{T}\|^2}\frac{\mathbf{U}'\mathbf{T}}{\|\mathbf{T}\|^2}\right\} \\ &= \operatorname{tr}\left(E\left\{\frac{\mathbf{U}\mathbf{U}'\mathbf{T}\mathbf{T}'}{\|\mathbf{T}\|^4}\right\}\right) \\ &= \operatorname{tr}\left(E\{\mathbf{U}\mathbf{U}'\}\, E\left\{\frac{\mathbf{T}\mathbf{T}'}{\|\mathbf{T}\|^4}\right\}\right) \\ &= \operatorname{tr}\left([\mathbf{I}_p + X_0^2\, \boldsymbol{\tau}\boldsymbol{\tau}']\, E\left\{\frac{\mathbf{T}\mathbf{T}'}{\|\mathbf{T}\|^4}\right\}\right) \\ &= E\left\{\frac{1}{\|\mathbf{T}\|^2}\right\} + X_0^2\, \boldsymbol{\tau}' E\left\{\frac{\mathbf{T}\mathbf{T}'}{\|\mathbf{T}\|^4}\right\} \boldsymbol{\tau}. \end{aligned} \tag{4.2}$$

As was mentioned in Section 2, there is a severe problem concerning the existence of the moments of the classical estimator, but the treatment of this problem is postponed to Section 6, where we will derive conditions under which the means involving **T** in (4.1) and (4.2) are finite. It is evident that these means, if they exist, will depend in some way on $\boldsymbol{\tau}$, as it is the only parameter in the distribution of **T**.

Our deductions in the next sections follow the lines of the proof of Lemma 11.3 as carried out by Arnold [1], although we consider our own approach more transparent, since we do not need an auxiliary conditional distribution. Moreover, Arnold does not provide an expression for the second mean in (4.2).

5. First and Second Moment in Terms of Noncentral Chi Squares

The starting point in this section is the normal distribution of **T**. We use this distribution to deduce the general results (5.3), (5.4), and (5.5), which we apply for $m=1$ and $m=2$. This will lead to alternative expressions for (4.1) and (4.2), which will be developed in the next section on the basis of the distribution of $\|\mathbf{T}\|^2$. We repeat that the existence of the moments will be justified in Section 6.

The probability density function of **T** is

$$f(\mathbf{t};\boldsymbol{\tau})=(2\pi)^{-p/2}\exp\left\{-\frac{\|\mathbf{t}-\boldsymbol{\tau}\|^2}{2}\right\},\quad \mathbf{t}=(t_1 t_2 \cdots t_p)',\ -\infty<t_i<\infty. \tag{5.1}$$

Let for $m=1, 2, \ldots$

$$\begin{aligned}E_{2m}&=E\left\{\frac{1}{\|\mathbf{T}\|^{2m}}\right\}\\&=\iint\cdots\int\frac{1}{\|\mathbf{t}\|^{2m}}f(\mathbf{t};\boldsymbol{\tau})\,dt_1\,dt_2\cdots dt_p.\end{aligned}\tag{5.2}$$

Consequently,

$$\frac{\partial}{\partial\tau_j}E_{2m}=\iint\cdots\int\frac{(t_j-\tau_j)}{\|\mathbf{t}\|^{2m}}f(\mathbf{t};\boldsymbol{\tau})\,dt_1\,dt_2\cdots dt_p. \tag{5.3}$$

If $i\neq j$ then

$$\frac{\partial^2}{\partial\tau_i\,\partial\tau_j}E_{2m}=\iint\cdots\int\frac{(t_i-\tau_i)(t_j-\tau_j)}{\|\mathbf{t}\|^{2m}}f(\mathbf{t};\boldsymbol{\tau})\,dt_1\,dt_2\cdots dt_p, \tag{5.4}$$

and if $i = j$ then

$$\frac{\partial^2}{\partial \tau_i \, \partial \tau_j} E_{2m} = \iint \cdots \int \frac{(t_i - \tau_i)(t_j - \tau_j)}{\|\mathbf{t}\|^{2m}} f(\mathbf{t}; \boldsymbol{\tau}) \, dt_1 \, dt_2 \cdots dt_p$$

$$- \iint \cdots \int \frac{1}{\|\mathbf{t}\|^{2m}} f(\mathbf{t}; \boldsymbol{\tau}) \, dt_1 \, dt_2 \cdots dt_p. \tag{5.5}$$

We may pull derivatives inside the integrals because the normal distribution is a member of an exponential family.

A compact notation for the vector of first-order partial derivatives is $\nabla(\cdot)$, where ∇ is the differential operator. For the matrix of second-order partial derivatives we use $\mathbf{H}(\cdot)$. It is readily seen from (5.3), (5.4), and (5.5) that the following equalities apply

$$\nabla(E_2) = E\left\{\frac{\mathbf{T} - \boldsymbol{\tau}}{\|\mathbf{T}\|^2}\right\}, \tag{5.6}$$

$$\nabla(E_4) = E\left\{\frac{\mathbf{T} - \boldsymbol{\tau}}{\|\mathbf{T}\|^4}\right\}, \tag{5.7}$$

$$\mathbf{H}(E_4) = E\left\{\frac{(\mathbf{T} - \boldsymbol{\tau})(\mathbf{T} - \boldsymbol{\tau})'}{\|\mathbf{T}\|^4}\right\} - \mathbf{I}_p E_4. \tag{5.8}$$

Elementary operations on the right of (5.6), (5.7), and (5.8) and substitution of the outcome thereof into (4.1) and (4.2) lead to

$$E\{\hat{X}_0\} = X_0[\boldsymbol{\tau}' \, \nabla(E_2) + \|\boldsymbol{\tau}\|^2 E_2], \tag{5.9}$$

and

$$E\{\hat{X}_0^2\} = E_2 + X_0^2[\boldsymbol{\tau}'\mathbf{H}(E_4)\, \boldsymbol{\tau} + 2\, \|\boldsymbol{\tau}\|^2 \boldsymbol{\tau}' \, \nabla(E_4)$$

$$+ (\|\boldsymbol{\tau}\|^2 + \|\boldsymbol{\tau}\|^4) E_4]. \tag{5.10}$$

The functions E_2 and E_4 in (5.9) and (5.10) are both means of functions of $\|\mathbf{T}\|^2$. Since $\mathbf{T}$ is normally distributed with mean $\boldsymbol{\tau}$ and covariance matrix $\mathbf{I}_p$, the variable $\|\mathbf{T}\|^2$ has a noncentral chi-squared distribution with p degrees of freedom and noncentrality parameter $\|\boldsymbol{\tau}\|^2$. Thus we have expressed the moments of the estimator in terms of noncentral chi squares.

6. First and Second Moment in Terms of Poisson Variables

In this section we reconsider the results (5.2) through (5.5) from a different starting point, namely the distribution of $\|\mathbf{T}\|^2$. Let

$$\lambda = \|\tau\|^2, \tag{6.1}$$

$$P(k, \lambda) = \frac{\exp(-\lambda/2)(\lambda/2)^k}{k!}, \tag{6.2}$$

$$G(p, k, \lambda) = \frac{y^{(p/2)+k-1}\exp(-y/2)}{\Gamma((p/2)+k)\,2^{(p/2)+k}}, \quad k = 0, 1, 2, \ldots; 0 < y < \infty. \tag{6.3}$$

The probability density function $g(y)$ of $\|\mathbf{T}\|^2$ is the noncentral chi-squared density function with p degrees of freedom and noncentrality parameter λ. This density function is as follows [1]

$$g(y) = \sum_k P(k, \lambda)\, G(p, k, y). \tag{6.4}$$

It is seen from (6.2) and (6.3) that this distribution is closely related to the Poisson distribution and the central chi-squared distribution.

Let E_{2m} be defined in (5.2). For $m = 1$ we get

$$\begin{aligned} E_2 &= \int \frac{1}{y} \sum_k P(k, \lambda)\, G(p, k, y)\, dy \\ &= \sum_k \frac{1}{p+2k-2} P(k, \lambda) \int G(p, k-1, y)\, dy. \end{aligned} \tag{6.5}$$

The integral in (6.5) exists for $(p/2) + k - 1 > 0$ and then the result is equal to 1, as it is the integral over a central chi-squared density function. Thus we find for $p > 2$

$$E_2 = E\left\{\frac{1}{p+2K-2}\right\}, \tag{6.6}$$

where $K \sim$ Poisson $(\lambda/2)$.

From similar arguments it is readily seen that for $p > 4$ the following applies

$$E_4 = E\left\{\frac{1}{(p+2K-2)(p+2K-4)}\right\}. \tag{6.7}$$

Throughout the rest of this section and in the next, we tacitly assume that K is a random variable with a Poisson distribution with parameter $\lambda/2$. It is seen again that the expressions for E_2 and E_4 are functions of τ, since the distribution of K depends on τ through λ. We find the analog of (5.6), (5.7), and (5.8) by partial differentiation of E_2 and E_4 with respect to the elements of τ. For brevity we restrict ourselves to the results of this procedure:

$$\nabla(E_2) = -2\,\tau E\left\{\frac{1}{(p+2K)(p+2K-2)}\right\}, \tag{6.8}$$

$$\nabla(E_4) = -4\,\tau E\left\{\frac{1}{(p+2K)(p+2K-2)(p+2K-4)}\right\}, \tag{6.9}$$

$$\begin{aligned} \mathbf{H}(E_4) = {} & 24\,\tau\tau' E\left\{\frac{1}{(p+2K+2)\cdots(p+2K-4)}\right\} \\ & -4\,\mathbf{I}_p E\left\{\frac{1}{(p+2K)(p+2K-2)(p+2K-4)}\right\}. \end{aligned} \tag{6.10}$$

Substitution in (5.9) and (5.10) leads to the following expressions for the moments. For $p > 2$,

$$E\{\hat{X}_0\} = X_0 E\left\{\frac{\lambda}{p+2K}\right\}, \tag{6.11}$$

and for $p > 4$

$$\begin{aligned} E\{\hat{X}_0^2\} = {} & E\left\{\frac{1}{p+2K-2}\right\} + X_0^2 E\left\{\frac{\lambda^2}{(p+2K+2)(p+2K)}\right\} \\ & + X_0^2 E\left\{\frac{\lambda}{(p+2K)(p+2K-2)}\right\}. \end{aligned} \tag{6.12}$$

Alternative expressions for (6.11) and (6.12) are

$$E\{\hat{X}_0\} = X_0\left[1 - E\left\{\frac{p-2}{p+2K-2}\right\}\right] \tag{6.13}$$

and

$$E\{\hat{X}_0^2\} = E\left\{\frac{1}{p+2K-2}\right\} + X_0^2 E\left\{\frac{2K(2K-1)}{(p+2K-2)(p+2K-4)}\right\}. \tag{6.14}$$

After some calculation we find for the mean squared error,

$$\begin{aligned} \mathrm{MSE}\{\hat{X}_0\} &= E\{(\hat{X}_0 - X_0)^2\} \\ &= E\left\{\frac{1}{p+2K-2}\right\} + X_0^2 E\left\{\frac{2K+(p-2)(p-4)}{(p+2K-2)(p+2K-4)}\right\}. \end{aligned} \tag{6.15}$$

7. Main Results and Approximations

We now return to the original problem, namely the estimation of x_0. In this section we combine the results from the preceding section with the reparametrization formulae given in Section 3. This leads to the two main expressions of this paper, (7.1) and (7.2). We also provide simple approximations for these exact results.

After some manipulation we find for $p > 2$,

$$E\{\hat{x}_0\} = x_0 - (x_0 - \bar{x})\, E\left\{\frac{p-2}{p+2K-2}\right\} \tag{7.1}$$

and for $p > 4$,

$$\begin{aligned} \mathrm{MSE}\{\hat{x}_0\} &= C\frac{n+1}{n}\, E\left\{\frac{1}{p+2K-2}\right\} \\ &\quad + (x_0 - \bar{x})^2\, E\left\{\frac{2K+(p-2)(p-4)}{(p+2K-2)(p+2K-4)}\right\}, \end{aligned} \tag{7.2}$$

where $K \sim$ Poisson $(\lambda/2)$,

$$\lambda = \|\tau\|^2 = C\, \boldsymbol{\beta}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\beta},$$

$$C = \sum_i (x_i - \bar{x})^2.$$

A Taylor expansion, the quadratic term included, leads to the approximation

$$E\left\{\frac{1}{p+2K-2}\right\} \approx \frac{1}{p+\lambda-2}\left\{1 + \frac{2\lambda}{(p+\lambda-2)^2}\right\}. \tag{7.3}$$

Figure 7.1 is a graphical representation of the exact and approximating values in (7.3) for $p = 3$, $p = 4$, and $p = 5$ as a function of λ. For $p > 5$ the approximations turned out to be graphically indistinguishable from the exact values, so we excluded them from the figure.

The quadratic term in the Taylor expansion is included because of the factor C in the first part of the mean squared error. In general, C is an increasing function of n, and for that reason Shukla [13] introduced a parameter σ_x^2

$$\begin{aligned} \sigma_x^2 &= \sum_i (x_i - \bar{x})^2/(n-1) \\ &= C/(n-1). \end{aligned} \tag{7.4}$$

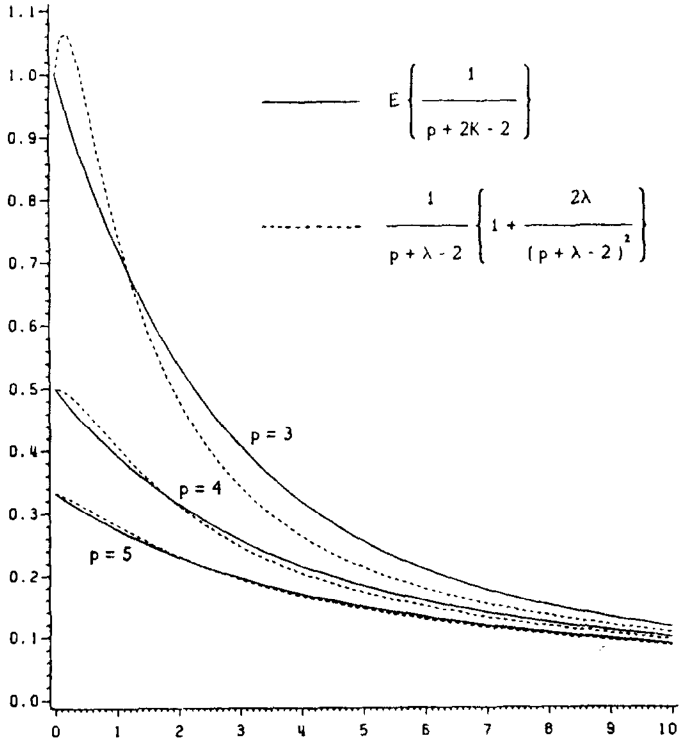

FIGURE 7.1

The value of σ_x^2 is thought to be more or less constant with increasing n, and this implies that λ is of order n. The factor $n+1$ in the numerator of the first part of mean squared error thus needs a λ^2 in the denominator to obtain an approximation of order $1/n$.

For large values of n the following simpler approximation can also be applied:

$$E\left\{\frac{1}{p+2K-2}\right\} \approx \frac{1}{\lambda}+\frac{4-p}{\lambda^2}. \tag{7.5}$$

This is readily derived from (7.3) by division, ignoring terms of the order $1/\lambda^3$.

Approximations to order $1/n$ for (7.1) and (7.2) are now

$$E\{\hat{x}_0\} \approx x_0-(x_0-\bar{x})\frac{p-2}{\lambda} \tag{7.6}$$

and

$$\mathrm{MSE}\{\hat{x}_0\} \approx \frac{1}{\boldsymbol{\beta}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\beta}}\left\{\frac{n+1}{n}+\frac{(x_0-\bar{x})^2}{C}+\frac{4-p}{\lambda}\right\}. \tag{7.7}$$

These expressions are in accordance with Shukla's results for $p=1$. As a check on (7.6) and (7.7) we extended Shukla's approach for multivariate observations, which gave the same results.

8. Conclusions

The mean and the mean squared error of a generalization of the classical estimator in multivariate calibration problems are given, both exact and approximative.

In this study it is assumed that the covariance matrix of the response vector is known, which will usually not be the case in practical situations. However, it is a good starting point in research which deals with the properties of multivariate calibration estimators.

In the field of multivariate calibration there are many open problems. For example, little is known about the distribution of the estimators for the unknown x_0. Also not investigated is the fact that multivariate observations, although done at unknown values of x, generally provide information concerning the parameters which are already estimated on the bases of the calibration experiment. Thus it must be possible in some way to update the estimates from the calibration experiment by means of the new observations. This is a remarkable difference between univariate and multivariate calibration problems.

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